

Quantum Complex Hénon-Heiles Potentials

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(February 1, 2008)

Abstract

Quantum-mechanical \mathcal{PT} -symmetric theories associated with complex cubic potentials such as $V = x^2 + y^2 + igxy^2$ and $V = x^2 + y^2 + z^2 + igxyz$, where g is a real parameter, are investigated. These theories appear to possess real, positive spectra. Low-lying energy levels are calculated to very high order in perturbation theory. The large-order behavior of the perturbation coefficients is determined using multidimensional WKB tunneling techniques. This approach is also applied to the complex Hénon-Heiles potential $V = x^2 + y^2 + ig(xy^2 - \frac{1}{3}x^3)$.

In this Letter we examine complex \mathcal{PT} -symmetric cubic Hamiltonians such as

$$\begin{aligned} H^{(2)} &\equiv p_x^2 + p_y^2 + x^2 + y^2 + igxy^2, \\ H^{(3)} &\equiv p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz, \end{aligned} \tag{1}$$

where g is a real parameter [1]. The superscript on H indicates the number of degrees of freedom; these Hamiltonians are several-degree-of-freedom generalizations of the one-dimensional complex cubic Hamiltonian $H^{(1)} = p^2 + x^2 + igx^3$, which has recently been studied in great detail by many authors [2–12]. The non-Hermitian Hamiltonian $H^{(1)}$ is interesting because its spectrum is entirely real and positive. The reality of the spectrum is apparently due to the \mathcal{PT} invariance of the Hamiltonian.

While many different one-degree-of-freedom examples of non-Hermitian \mathcal{PT} -symmetric quantum systems have been studied, no multidimensional complex \mathcal{PT} -symmetric coupled-oscillator systems have been examined. The purpose of this Letter is to show that (i) the property of real, positive spectra persists even for quantum systems having several degrees of freedom, and (ii) these theories have many other properties in common with theories described by conventional Hermitian Hamiltonians.

Direct numerical evidence for the reality and positivity of the spectrum of $H^{(1)}$ can be found by performing a Runge-Kutta integration of the associated complex Schrödinger equation [2]. Alternatively, the large-energy eigenvalues of the spectrum can be calculated with great accuracy by using conventional WKB techniques [13]. A strong argument for the reality and positivity of the spectrum can be obtained by calculating the spectral zeta function $Z(1)$ (the sum of the inverses of the eigenvalues). For the Hamiltonian¹ $H = p^2 + ix^3$ this was done by Mezincescu [8] and Bender and Wang [10]. The exact result for $Z(1)$ is

$$Z(1) = \frac{4 \sin^2(\pi/5) \Gamma^2(1/5)}{5^{6/5} \Gamma(3/5)}. \quad (2)$$

Using the numerical values of the first few eigenvalues and the WKB formula for the high eigenvalues, one can conclude that any complex eigenvalues must be larger in magnitude than about 10^{18} . Some rigorous results regarding the reality of the eigenvalues of $H^{(1)}$ have been obtained by Shin [11], who showed that the entire spectrum must lie in a narrow wedge containing the positive-real axis. Other results have been obtained by Delabaere *et al* [3,7].

Let us now return to the Hamiltonians in (1). The Schrödinger equations associated with $H^{(1)}$, $H^{(2)}$, and $H^{(3)}$ are

$$-\psi_1''(x) + (x^2 + igx^3)\psi_1(x) = E\psi_1(x),$$

¹This Hamiltonian, the *massless* case of $H^{(1)}$, has a positive discrete spectrum. It is not known if the massless versions of $H^{(2)}$ and $H^{(3)}$ have discrete spectra. Indeed, even for the massless coupled anharmonic oscillator potential $V = x^2y^2$, it is also not known if the spectrum is discrete.

$$\begin{aligned}
-\nabla^2\psi_2(x, y) + (x^2 + y^2 + igxy^2)\psi_2(x, y) &= E\psi_2(x, y), \\
-\nabla^2\psi_3(x, y, z) + (x^2 + y^2 + z^2 + igxyz)\psi_3(x, y, z) &= E\psi_3(x, y, z).
\end{aligned} \tag{3}$$

We have solved the Schrödinger equations (3) for the eigenvalues in several ways. One technique is to diagonalize each Hamiltonian in a set of multidimensional harmonic oscillator basis states. This procedure immediately reveals that the energy levels are real.

A more precise calculation of the energies of the complex \mathcal{PT} -symmetric Hamiltonians in (1) is performed using high-order Rayleigh-Schrödinger perturbation theory. This technique was used in Refs. [6] and [12] to obtain the perturbation series for the ground-state energy of $H^{(1)}$. In these references it was found that the Rayleigh-Schrödinger perturbation series is Borel summable and that Padé summation is in excellent agreement with the real energy spectrum. Furthermore, Padé analysis provides strong numerical evidence that the once-subtracted ground-state energy considered as a function of g^2 is a Stieltjes function.

The Rayleigh-Schrödinger perturbation series for the ground-state energies $E_0^{(1)}$, $E_0^{(2)}$, and $E_0^{(3)}$ of the Hamiltonians $H^{(1)}$, $H^{(2)}$, and $H^{(3)}$ have the asymptotic form

$$\begin{aligned}
E_0^{(1)} &\sim 1 + \frac{11}{16}g^2 - \frac{465}{256}g^4 + \frac{39709}{4096}g^6 - \frac{19250805}{262144}g^8 + \frac{2944491879}{4194304}g^{10} + \dots, \\
E_0^{(2)} &\sim 2 + \frac{5}{48}g^2 - \frac{223}{6912}g^4 + \frac{114407}{4976640}g^6 - \frac{346266143}{14332723200}g^8 + \frac{2360833242959}{72236924928000}g^{10} + \dots, \\
E_0^{(3)} &\sim 3 + \frac{1}{48}g^2 - \frac{7}{4608}g^4 + \frac{5069}{19906560}g^6 - \frac{2441189}{38220595200}g^8 \\
&\quad + \frac{8034211571}{385263599616000}g^{10} + \dots
\end{aligned} \tag{4}$$

in the limit $g \rightarrow 0$. The (9, 9) Padé was constructed from the once-subtracted form of these series and the results are plotted in Fig. 1. The first two excited states of $H^{(2)}$ are plotted in Fig. 2. Note that the degenerate unperturbed energy level at $E = 4$ splits into two levels, each of which is greater than four.

The perturbation coefficients in these series are derived from recursion relations like those first derived for the anharmonic oscillator [14]. These recursion relations are obtained directly from the Schrödinger equations (3). We substitute $\psi_1(x) = e^{-x^2/2}\phi_1(x)$, $\psi_2(x, y) = e^{-(x^2+y^2)/2}\phi_2(x, y)$ and $\psi_3(x, y, z) = e^{-(x^2+y^2+z^2)/2}\phi_3(x, y, z)$, where $\phi_{1,2,3}$ are formal power

series in g ; the coefficients of g^n are polynomials P_n of degree $3n$ in the variables x, y, z . For example, for the case of ψ_3 , $P_n = \sum_{j,k,l=0}^n a_{n,j,k,l} x^j y^k z^l$, and the coefficients $a_{n,j,k,l}$ satisfy

$$a_{n,j,k,l} = \frac{1}{2(j+k+l)} \left[a_{n-1,j-1,k-1,l-1} - 2 \sum_{p=1}^{n-1} a_{n-p,j,k,l} (a_{p,2,0,0} + a_{p,0,2,0} + a_{p,0,0,2}) \right. \\ \left. + (j+1)(j+2)a_{n,j+2,k,l} + (k+1)(k+2)a_{n,j,k+2,l} + (l+1)(l+2)a_{n,j,k,l+2} \right]. \quad (5)$$

Once the coefficients $a_{n,j,k,l}$ are known, we can construct the coefficient of g^{2n} in the expansion for the ground-state energy $E_0^{(3)}$ in (4) according to

$$E_0^{(3)} \sim 3 + 2 \sum_{n=1}^{\infty} (a_{2n,2,0,0} + a_{2n,0,2,0} + a_{2n,0,0,2}) (-g^2)^n \quad (g \rightarrow 0). \quad (6)$$

We are particularly interested in the large-order behavior of the coefficients in the perturbation expansion because this behavior suggests that the series is Borel summable and reveals the analytic structure of the energy level as a function of complex g^2 . In Ref. [6] it is shown that the large- n behavior of the coefficient of g^{2n} in the expansion of $E_0^{(1)}$ is

$$(-1)^{n+1} \frac{4}{\pi^{3/2}} \left(\frac{15}{8} \right)^{n+1/2} \Gamma \left(n + \frac{1}{2} \right) \left[1 - O \left(\frac{1}{n} \right) \right] \quad (n \rightarrow \infty). \quad (7)$$

Therefore, although divergent, the series for $E_0^{(1)}$ is Borel summable [13]. Observe that if the factor of i were absent from the Hamiltonian $H^{(1)}$, then the perturbation coefficients would not alternate in sign and the perturbation series would not be Borel summable.

A major result reported here is the large-order behavior of the coefficients of g^{2n} in the series for $E_0^{(2)}$

$$(-1)^{n+1} \frac{72\sqrt{2}}{\pi \sqrt{\cosh(\frac{1}{2}\pi\sqrt{23})}} \left(\frac{5}{18} \right)^{n+1/2} \Gamma \left(n + \frac{1}{2} \right) \left[1 - O \left(\frac{1}{n} \right) \right] \quad (n \rightarrow \infty), \quad (8)$$

and coefficients of g^{2n} in the series for $E_0^{(3)}$

$$(-1)^{n+1} \frac{1152\sqrt{3}}{\sqrt{\pi} \cosh(\frac{1}{2}\pi\sqrt{23})} \left(\frac{5}{72} \right)^{n+1/2} \Gamma \left(n + \frac{1}{2} \right) \left[1 - O \left(\frac{1}{n} \right) \right] \quad (n \rightarrow \infty). \quad (9)$$

We have verified these results to extremely high precision by performing a Richardson extrapolation [13] of the perturbation coefficients in (4) divided by these behaviors.

We derive these results by adapting the multidimensional WKB tunneling techniques in Ref. [15]. We observe that if g is replaced by ig in $H^{(2)}$ and $H^{(3)}$, then we obtain potentials for which the probability current in a Gaussian ground state leaks out to infinity. The probability flows outward along most-probable escape paths (MPEPs).

To determine the MPEPs for $H^{(2)}$ we rewrite the potential in polar coordinates:

$$V(x, y) = x^2 + y^2 - gxy^2 = r^2 - gr^3 \cos \theta \sin^2 \theta, \quad (10)$$

where $x = r \cos \theta$, $y = r \sin \theta$. Letting $\alpha = g \cos \theta \sin^2 \theta$, we calculate $V_r = 2r - 3\alpha r^2$. Then, setting $V_r = 0$ gives the critical radius $r = \frac{2}{3\alpha}$, and at this radius the potential has the value $\frac{4}{27}\alpha^{-2}$. Thus, V achieves its minimum when $\sin \theta = \pm\sqrt{\frac{2}{3}}$. Therefore, the effective radial potential is $V(r) = r^2 - \frac{2g}{3\sqrt{3}}r^3$. We conclude that there are two straight-line MPEPs symmetrically placed above and below the positive- x axis (see Fig. 3).

Geometrical optics (ray tracing) is sufficient to reproduce the gamma-function and exponential behaviors in (8). We simply evaluate the approximate WKB integral

$$I = -2 \int_0^{\frac{3\sqrt{3}}{2g}} dr \sqrt{r^2 - \frac{2g}{3\sqrt{3}}r^3},$$

where we have neglected the constant term in the limit of small g . We evaluate the resulting beta-function integral to get the leading exponent in the tunneling rate: $I = -\frac{18}{5}g^{-2}$. There is a standard dispersion-integral procedure [6,14] that expresses the large-order behavior as the n th inverse moment of the tunneling rate. This procedure gives the behavior in (8) apart from an overall multiplicative constant. This constant can only be determined by performing a *physical-optics* calculation of the tunneling rate.

For this physical-optics calculation we must determine the flux of probability through a tube centered about the MPEP. We introduce a rotated coordinate system by

$$x = \frac{1}{\sqrt{3}}r - \frac{\sqrt{2}}{\sqrt{3}}t, \quad y = \frac{1}{\sqrt{3}}t + \frac{\sqrt{2}}{\sqrt{3}}r,$$

so that r measures the distance along the MPEP and t is the coordinate transverse to the MPEP. In terms of these variables, the Schrödinger equation (3) for ψ_2 reads

$$-\nabla^2\psi_2(r,t) + \left[r^2 + t^2 + \frac{g}{3\sqrt{3}}(-2r^3 + 3rt^2 - \sqrt{3}t^3) - 2 \right] \psi_2(r,t) = 0, \quad (11)$$

where we have replaced g by ig . We may drop the t^3 term because $gt^3 \ll t^2$ for small g .

Next, we separate the radial dependence from the transverse dependence by writing $\psi_2(r,t) = W(r)\phi(r,t)$. The function $W(r)$, which expresses the radial dependence, satisfies the differential equation $W''(r) = \left(r^2 - \frac{2g}{3\sqrt{3}}r^3 - 1 \right) W(r)$. The WKB approximation to the decaying solution to this equation is

$$W(r) = \frac{e^{-1/4} \exp \left(- \int_1^r ds \sqrt{s^2 - \frac{2g}{3\sqrt{3}}s^3 - 1} \right)}{\sqrt{2} \left(r^2 - \frac{2g}{3\sqrt{3}}r^3 - 1 \right)^{1/4}}, \quad (12)$$

where the numerical factors are included in anticipation of asymptotic matching. The equation for $\phi(r,t)$ is $-2\frac{W_r}{W}\phi_r - \phi_{rr} - \phi_{tt} + (t^2 + \frac{g}{\sqrt{3}}rt^2 - 1)\phi = 0$. Note that $W_r/W \sim -r$ for small g . The change of variable $v = \sqrt{1 - \frac{2g}{3\sqrt{3}}r}$ yields a parabolic equation for ϕ :

$$(v^2 - 1)\phi_v - \phi_{tt} + [t^2 + 3t^2(1 - v^2)/2 - 1]\phi = 0, \quad (13)$$

where we neglect the small term of order $g^2\phi_{vv}$. The solution to this equation has the form of a Gaussian that expresses the thickness of the stream of probability current that flows outward along the MPEP:

$$\phi(v,t) = A(v)e^{-t^2 f(v)/2}, \quad (14)$$

where the function $f(v)$ satisfies the Riccati equation

$$(1 - v^2)f'(v) - 2f^2(v) + 5 - 3v^2 = 0 \quad (15)$$

and $A(v)$ satisfies the transport equation

$$(1 - v^2)A'(v) - f(v)A(v) + A(v) = 0. \quad (16)$$

To solve the Riccati equation (15) we substitute $f(v) = -\frac{1}{2}(1 - v^2)h'(v)/h(v)$ and convert it to the second-order linear equation

$$(1 - v^2)h''(v) - 2vh'(v) + \left(-6 - \frac{4}{1 - v^2} \right) h(v) = 0, \quad (17)$$

which we recognize as the Legendre differential equation [16].

To find the initial conditions on $f(v)$ and $A(v)$, we match $\phi(v, t)$ to the wave-function solution to the Schrödinger equation (11) in the inner region where r and t are of order 1. In this region the wave function is a Gaussian: $\phi(v, t) = e^{-(r^2+t^2)/2}$. By construction, for small r , $W(r) \sim e^{-r^2/2}$. Thus, we obtain the initial conditions $A(1) = 1$ and $f(1) = 1$. Hence, the solution to (17) is the Legendre function $h(v) = P_\nu^{-2}(v)$, where $\nu(\nu + 1) = -6$.

Our objective now is to find the flux of probability at the distant turning point [15]. At this turning point the radial component of the probability current is

$$J = 2 \frac{1}{2\sqrt{e}} e^{-t^2 f(0)} A^2(0) \exp \left(-2 \int_1^{\frac{3\sqrt{3}}{2g}} ds \sqrt{s^2 - \frac{2g}{3\sqrt{3}} s^3 - 1} \right), \quad (18)$$

where we have included a factor of 2 because there are two channels. We integrate in the transverse direction to get the total flux of probability current $\int_{-\infty}^{\infty} dt e^{-t^2 f(0)} = \sqrt{\frac{\pi}{f(0)}}$ and we evaluate the integral in the exponent to obtain

$$2 \int_1^{\frac{3\sqrt{3}}{2g}} ds \sqrt{s^2 - \frac{2g}{3\sqrt{3}} s^3 - 1} \sim \frac{18}{5g^2} - \ln(12\sqrt{3}) + \ln(g) - \frac{1}{2} \quad (g \rightarrow 0).$$

Thus, the total outward flux of probability is $\frac{12\sqrt{3}}{g} A^2(0) \sqrt{\frac{\pi}{f(0)}} e^{-18/(5g^2)}$. Substituting this result into the dispersion integral, we obtain the following formula for the large-order behavior of the coefficients in the perturbation series for the ground-state energy:

$$(-1)^{n+1} \frac{12A^2(0)\sqrt{3}}{\pi\sqrt{\pi f(0)}} \left(\frac{5}{18}\right)^{n+1/2} \Gamma\left(n + \frac{1}{2}\right) \left[1 - O\left(\frac{1}{n}\right)\right] \quad (n \rightarrow \infty). \quad (19)$$

It remains to find the numbers $f(0)$ and $A(0)$. Using the hypergeometric-function representation for the Legendre function [16], we obtain

$$f(0) = -\tan(\pi\nu/2) \frac{\Gamma(\nu/2)\Gamma(2+\nu/2)}{\Gamma(-1/2+\nu/2)\Gamma(3/2+\nu/2)}$$

and

$$A(0) = \pi^{-1/4} \sqrt{2\Gamma(2+\nu/2)\Gamma(3/2-\nu/2)}.$$

Thus, $A^2(0)/\sqrt{f(0)} = \sqrt{24\pi/\cosh(\pi\sqrt{23}/2)}$ and we have derived the result in (8).

To obtain the formula (9) we follow the same procedure. In this case there are four radial MPEPs and there are two transverse variables. We begin by introducing a change of coordinates in the Schrödinger equation (3) for $\psi_3(x, y, z)$:

$$x = \frac{1}{\sqrt{3}}r + \frac{1}{\sqrt{6}}s - \frac{1}{\sqrt{2}}t, \quad y = \frac{1}{\sqrt{3}}r + \frac{1}{\sqrt{6}}s + \frac{1}{\sqrt{2}}t, \quad z = \frac{1}{\sqrt{3}}r - \frac{2}{\sqrt{6}}s.$$

The remainder of the calculation is identical to that summarized above for $\psi_2(x, y)$.

We conclude by noting that the complex Hénon-Heiles potential

$$V^{HH} = x^2 + y^2 + ig(xy^2 - \frac{1}{3}x^3) \tag{20}$$

has a Borel summable Rayleigh-Schrödinger perturbation series for the ground-state energy, with the leading growth of the coefficients given by

$$C(-1)^{n+1} \left(\frac{5}{24}\right)^{n+1/2} \Gamma\left(n + \frac{1}{2}\right) \left[1 + O\left(\frac{1}{n}\right)\right] \quad (n \rightarrow \infty), \tag{21}$$

where C is a constant. A simple geometric-optics calculation (with g replaced by ig) confirms this leading growth rate. There are three MPEPs, a pair of MPEPs similar to those encountered in our analysis of $H^{(2)}$ (now at angles $\pm\frac{\pi}{3}$ from the positive- x axis), and a third MPEP along the negative- x axis, which is like that for $H^{(1)}$ (see Fig. 4). Remarkably, these two different types of MPEPs produce exactly the same leading contribution to (21). This fact depends crucially on having the appropriate combinatorial factors in (20).

Finally, we remark that the quantum field theoretic generalizations of the Hamiltonians studied here, particularly $H^{(2)}$, may be viewed as theories of scalar electrodynamics. It would be interesting to study such issues as bound states and Schwinger-Dyson equations in such theories.

ACKNOWLEDGMENTS

MŞ is grateful to the Physics Department at Washington University for their hospitality during his sabbatical. This work was supported by the U.S. Department of Energy.

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FIGURES

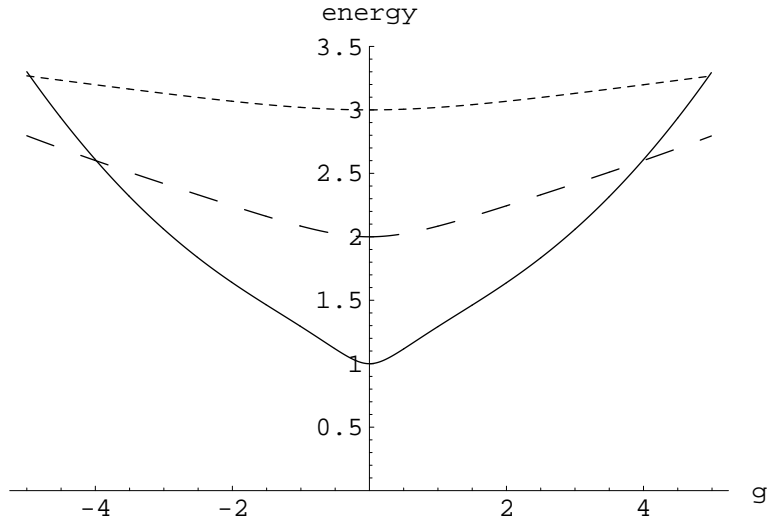


FIG. 1. Ground-state energies of the Hamiltonians $H^{(1)}$ (solid line), $H^{(2)}$ (long-dashed line), and $H^{(3)}$ (short-dashed line), as functions of the coupling constant g . Note that the energy levels are real and positive. The graphs were obtained from the (9,9) Padé constructed from the once-subtracted perturbation series for these energy levels.

FIGURE 2

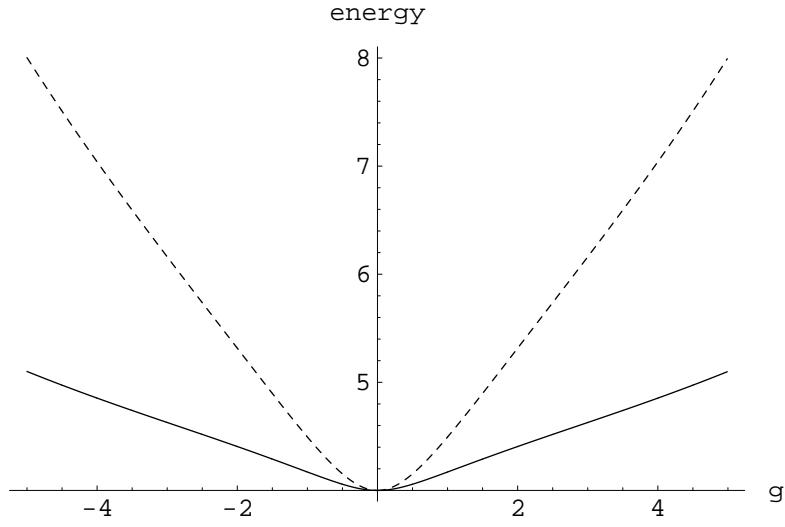


FIG. 2. First two excited energies of the Hamiltonian $H^{(2)}$. The solid and dashed lines represent the levels whose unperturbed states are $xe^{-(x^2+y^2)/2}$ and $ye^{-(x^2+y^2)/2}$. The unperturbed energies split into two distinct levels, both of which lie above the unperturbed level at $E = 4$. The graphs were constructed from the (9,9) Padé of the perturbation expansion in powers of g^2 .

FIGURE 3

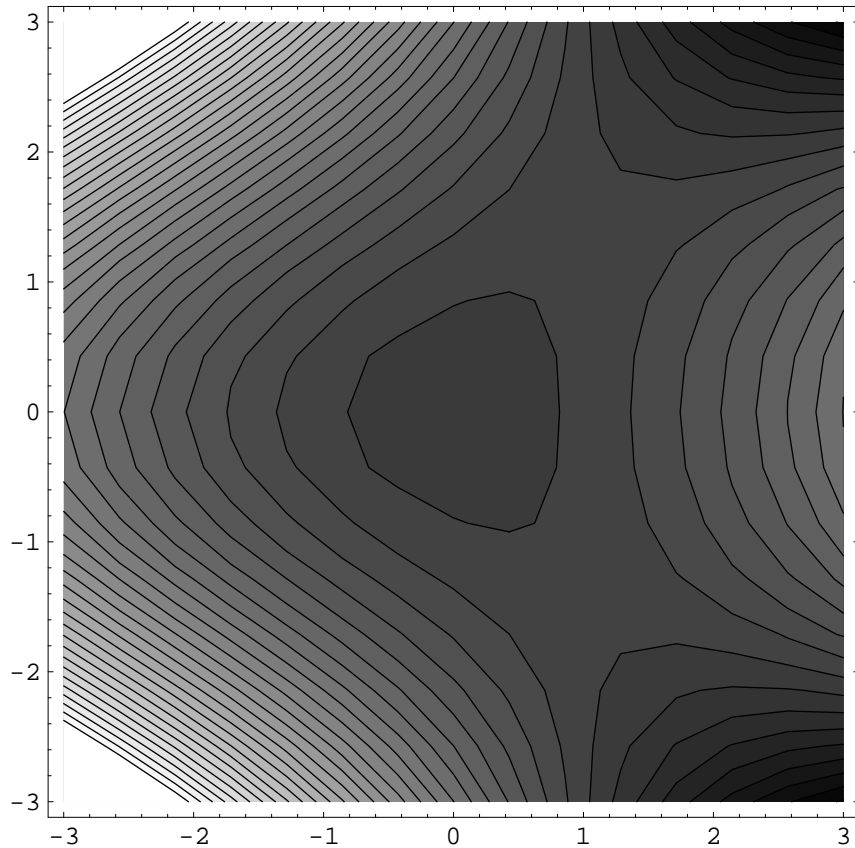


FIG. 3. Contour plot of the potential $x^2+y^2-xy^2$. A Gaussian probability distribution localized at the origin gradually leaks out to infinity preferentially along two channels in the right-half plane. These channels are called most probable escape paths (MPEPs).

FIGURE 4

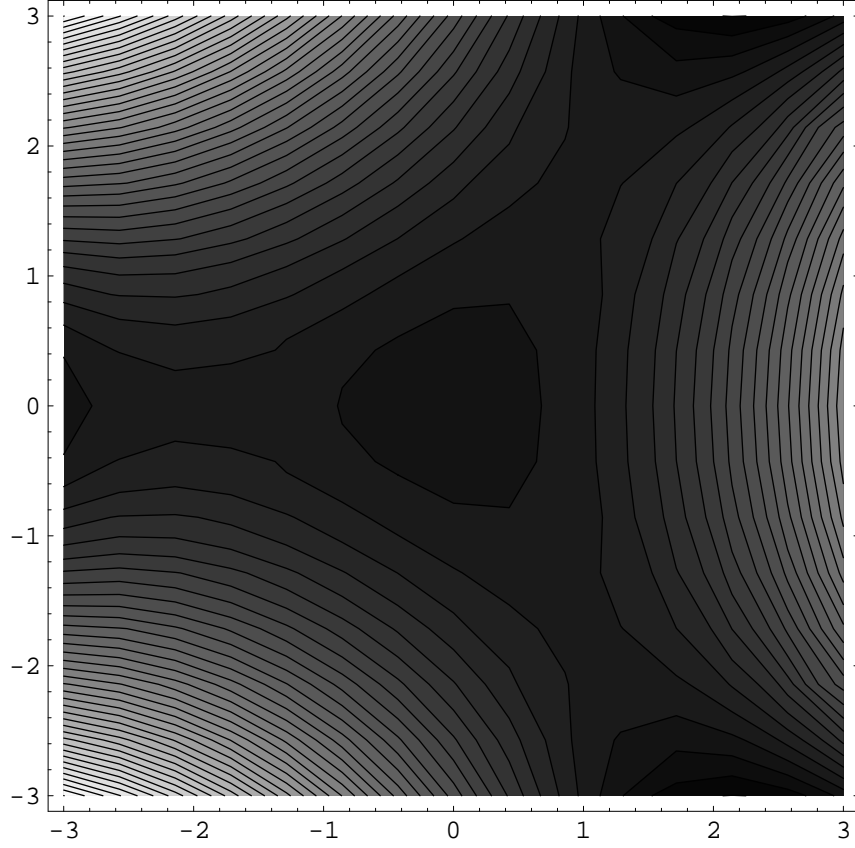


FIG. 4. Contour plot of the Hénon-Heiles potential $x^2 + y^2 - xy^2 + \frac{1}{3}x^3$. A Gaussian probability distribution localized at the origin tunnels out to infinity preferentially along three MPEPs, two in the right-half plane and one along the negative-real axis. Remarkably, the contribution from all three MPEPs to the large-order behavior of perturbation theory is of the same magnitude.